

## QUANTUM CHEMICAL STUDY OF THE REACTION OF $C^+$ WITH INTERSTELLAR ICE: PREDICTIONS OF VIBRATIONAL AND ELECTRONIC SPECTRA OF REACTION PRODUCTS

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The  $C^+$  cation (CII) is the dominant form of carbon in diffuse clouds and an important tracer for star formation in molecular clouds. We studied the low energy deposition of  $C^+$  on ice using density functional theory calculations on water clusters as large as 18  $H_2O$ . Barrierless reactions occur with water to form two dominant sets of products:  $HOC + H_3O^+$  and  $CO^- + 2H_3O^+$ . In order to provide testable predictions, we have computed both vibrational and electronic spectra for pure ice and processed ice clusters. While vibrational spectroscopy is expected to be able to discern that  $C^+$  has reacted with ice by the addition of  $H_3O^+$  features not present in pure ice, it does not provide characteristic bands that would discern between  $HOC$  and  $CO^-$ . On the other hand, predictions of electronic spectra suggest that low energy absorptions may occur for  $CO^-$  and not  $HOC$ , making it possible to distinguish one product from the other.